1. Notes

2. Result Statistics

Figure 1. False discovery rate (FDR) curve. X axis is the number of peptide-spectrum matches (PSM) being kept. Y axis is the corresponding FDR. ❷
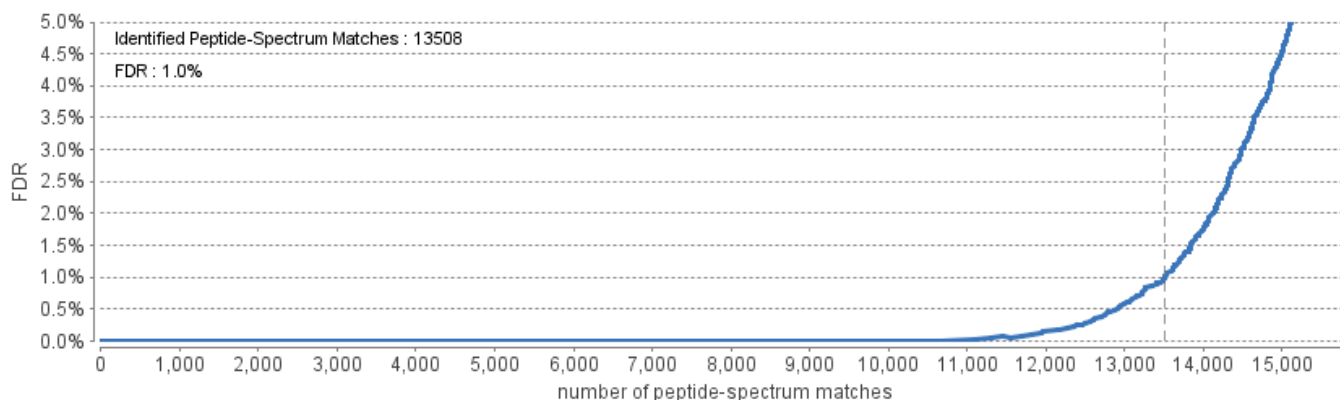

Figure 2. PSM score distribution. **(a)** Distribution of PEAKS peptide score; **(b)** Scatterplot of PEAKS peptide score versus precursor mass error. ❷

(a)   **(b)**
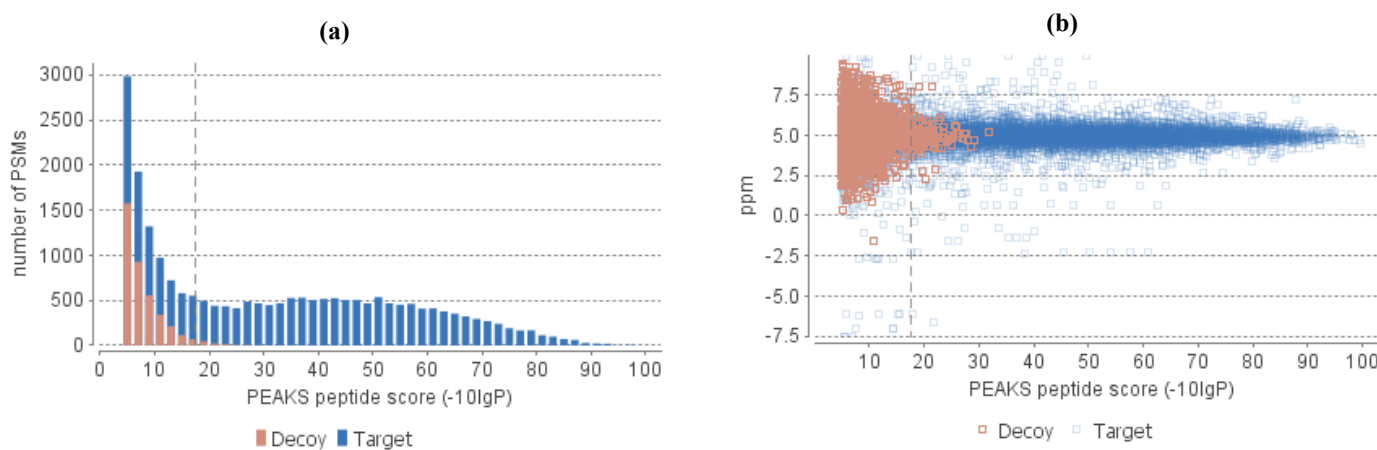

Figure 3. De novo result validation. Distribution of residue local confidence: **(a)** Residues in de novo sequences validated by confident database peptide assignment; **(b)** Residues in "de novo only" sequences. ❷
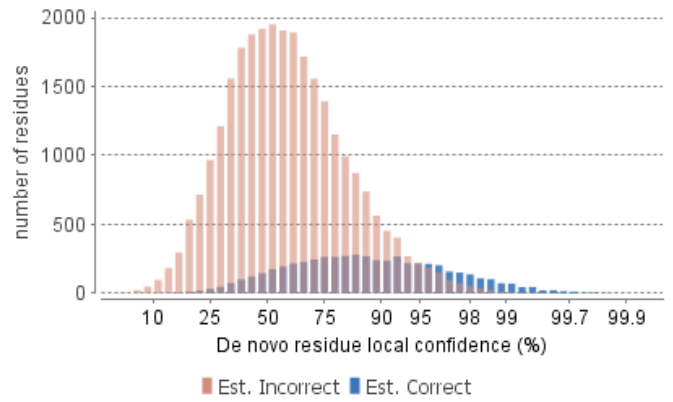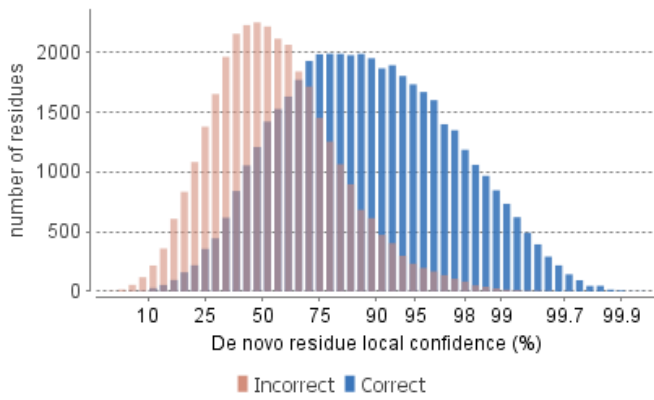
(a)   **(b)**

| | | | Incorrect | Correct | | | | | Est. Incorrect | Est. Correct |

Table 1. Statistics of data.

# of MS Scans	0
# of MS/MS Scans	40553

Table 2. Result filtration parameters.

Peptide -10lgP	≥17.6
Protein -10lgP	≥20
Proteins unique peptides	≥1
De novo ALC Score	≥50%

Table 3. Statistics of filtered result.

Peptide-Spectrum Matches	13508
Peptide Sequences	6227
Protein Groups	1040
Proteins	1769
Proteins (#Unique Peptides)	806 (>2); 431 (=2); 532 (=1);
FDR (Peptide-Spectrum Matches)	1.0%
FDR (Peptide Sequences)	2.0%
FDR (Protein)	0.0%
De Novo Only Spectra	3029

Table 4. PTM profile.

Name	ΔMass	#PSM	Position
Carbamidomethyl	57.02	1766	C
Oxidation	15.99	1185	M
Acetylation	42.01	243	Protein N-term

3. Experiment Control

Figure 4. Precursor mass error of peptide-spectrum matches (PSM) in filtered result. **(a)** Distribution of precursor mass error in ppm; **(b)** Scatterplot of precursor m/z versus precursor mass error in ppm.
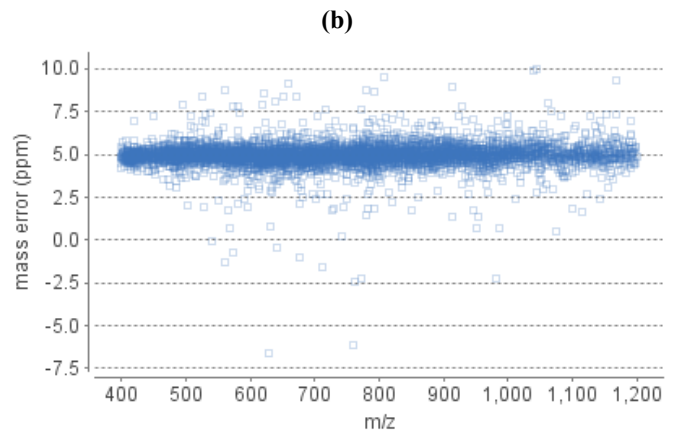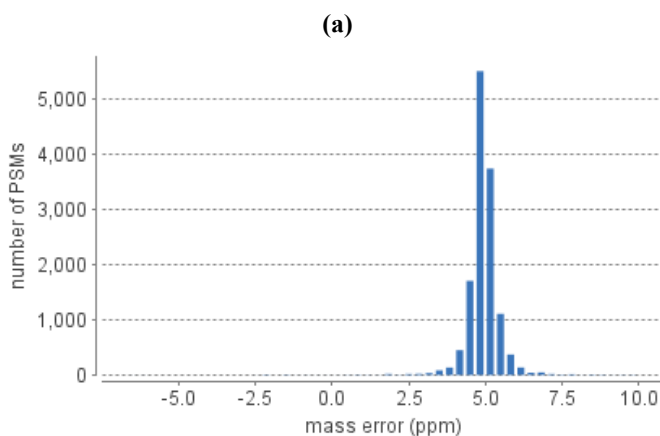
(a)

(b)

Table 5. Number of identified peptides in each sample by the number of missed cleavages

Missed Cleavages	0	1	2	3	4+
Sample 1	3467	2144	603	11	2

4. Other Information

Table 6. Search parameters.
Query Type: Homology Match
Fixed Modifications:
  Carbamidomethylation: 57.02
Variable Modifications:
  Oxidation (M): 15.99
  Acetylation (Protein N-term): 42.01
Fragment ion tolerance: 0.5
L equals I: true
Q equals K: true
Report number: 1
Maximum # of PTMs: 5
De novo score (ALC%) threshold: 15
Peptide hit threshold (-10logP): 30.0
Peaks run ID: 3
Merge Options: no merge
Precursor Options: corrected
Charge Options: no correction
Filter Quality: >0.65
Process: true

Protein List

Table 7. Instrument parameters.
Fractions: Progenesis _to_Peaks_ASTRUS..mgf
Ion Source: ESI(nano-spray)
Fragmentation Mode: CID, CAD(y and b ions)
MS Scan Mode: FT-ICR/Orbitrap
MS/MS Scan Mode: Linear Ion Trap